FORM PTO-1449

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0870001	APPLICATION NO. 09/814,160
APPLICANT Agrafiotis et al.	
FILING DATE March 22, 2001	GROUP 2122

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
Haw	AA1	4,773,099	09/1988	Bokser	382	14	
	AB1	4,811,217	03/1989	Tokizane et al.	364	300	
	AC1	4,859,736	08/1989	Rink	525	54.1	
	AD1	4,908,773	03/1990	Pantoliano et al.	364	496	
	AE1	4,935,875	06/1990	Shah et al.	364	497	
	AF1	4,939,666	07/1990	Hardman	364	496	
	AG1	5,010,175	04/1991	Rutter et al.	530	334	
	AH1	5,025,388	06/1991	Cramer, III et al.	364	496	
	AI1	5,155,801	10/1992	Lincoln	395	22	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
Haw	AJ1	EP 0 355 266 B1	02/1990	EPO	B01J	19/00	Yes No
	AK1	EP 0 355 628 B1	02/1990	EPO	G21F	9/00	Yes No
	AL1	EP 0 770 876 A1	05/1997	EPO	G01N	33/68	Yes No
	AM1	EP 0 818 744 A2	01/1998	EPO	G06F	17/50	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

Haw	AN	1	Borg, Ingwer and Groenen, Patrick, *Modern Multidimensional Scaling Theory and Applications*, Springer Series in Statistics, 1997, entire book submitted.
	AO	1	Agrafiotis, D.K. *et al.*, "Advances in diversity profiling and combinatorial series design," *Molecular Diversity*, Kluwer Academic Publishers, Vol. 4, 1999, pp. 1-22.
	AP	1	Agrafiotis, D.K. and Lobanov, V.S., "An Efficient Implementation of Distance-Based Diversity Measures Based on k-d Trees," *J. Chem. Inf. Comput. Sci.*, American Chemical Society, Vol. 39, No. 1, January/February 1999, pp. 51-58.
	AQ	1	Agrafiotis, D.K. and Lobanov, V.S., "Bridging The Gap Between Diversity And QSAR," *Abstracts of Papers Part 1: 215th ACS National Meeting*, March 29-April 2, 1998, p. 181-COMP.
	AR	1	Agrafiotis, D.K. and Jaeger, E.P., "Directed Diversity®: An Operating System For Combinatorial Chemistry," *Abstracts of Papers Part 1: 211th ACS National Meeting*, March 24-28, 1996, p. 46-COMP.

EXAMINER *Hoangan Cu Mg Nguyen*	DATE CONSIDERED 5/14/04

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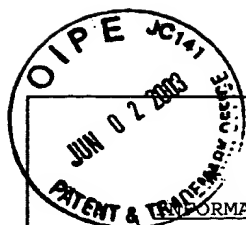
ATTY. DOCKET NO. 1503.0870001	APPLICATION NO. 09/814,160
APPLICANT Agrafiotis et al.	
FILING DATE March 22, 2001	GROUP 2122

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
Han	AA2	5,167,009	11/1992	Skeirik	395	27	
	AB2	5,181,259	01/1993	Rorvig	382	36	
	AC2	5,240,680	08/1993	Zuckermann et al.	422	67	
	AD2	5,260,882	11/1993	Blanco et al.	364	499	
	AE2	5,265,030	11/1993	Skolnick et al.	364	496	
	AF2	5,270,170	12/1993	Schatz et al.	435	7.37	
	AG2	5,288,514	02/1994	Ellman	427	2	
	AH2	5,307,287	04/1994	Cramer, III et al.	364	496	
	AI2	5,323,471	06/1994	Hayashi	382	15	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
Han	AJ2	WO 91/19735	12/1991	PCT	C07K	7/02	Yes No
	AK2	WO 92/00091	01/1992	PCT	A61K	37/02	Yes No
	AL2	WO 93/20242	10/1993	PCT	C12Q	1/70	Yes No
	AM2	WO 94/28504	12/1994	PCT	G06F	15/60	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

|		
Han	AN	2	Agrafiotis, D.K., "Diversity of Chemical Libraries," *Encyclopedia of Computational Chemistry*, John Wiley & Sons Ltd, Vol. 1:A-D, 1998, pp. 742-761.
	AO	2	Agrafiotis, D.K., "On the Use of Information Theory for Assessing Molecular Diversity," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 3, May/June 1997, pp. 576-580.
	AP	2	Agrafiotis, D.K. *et al.*, "Parallel QSAR," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 50-COMP.
	AQ	2	Agrafiotis, D.K. *et al.*, "PRODEN: A New Program for Calculating Integrated Projected Populations," *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 11, No. 9, October 1990, pp. 1101-1110.
	AR	2	Agrafiotis, D.K. and Jaeger, E.P., "Stochastic Algorithms for Exploring Molecular Diversity," *Abstracts of Papers Part 1: 213th ACS National Meeting*, April 13-17, 1997, p. 16-CINF.

EXAMINER Hoang guy Anthony Nguyen Ba	DATE CONSIDERED 5/14/04

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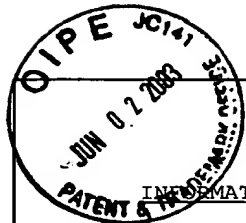
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ATTY. DOCKET NO. 1503.0870001		APPLICATION NO. 09/814,160
APPLICANT Agrafiotis et al.		
FILING DATE March 22, 2001		GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
Han	AA3	5,331,573	07/1994	Balaji et al.	364	500	
	AB3	5,434,796	07/1995	Weininger	364	496	
	AC3	5,436,850	07/1995	Eisenberg et al.	364	496	
	AD3	5,442,122	08/1995	Noda et al.	564	426	RECEIVED
	AE3	5,463,564	10/1995	Agrafiotis et al.	364	496	
	AF3	5,499,193	03/1996	Sugawara et al.	364	500	JUN 0 3 2003
	AG3	5,519,635	05/1996	Miyake et al.	364	497	
	AH3	5,524,065	06/1996	Yagasaki	382	226	Technology Center 2100
	AI3	5,526,281	06/1996	Chapman et al.	364	496	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
Han	AJ3	WO 95/01606	01/1995	PCT	G06F	15/42	Yes No
	AK3	WO 97/09342	03/1997	PCT	C07H	21/02	Yes No
	AL3	WO 97/20952	06/1997	PCT	C12Q	1/68	Yes No
	AM3	WO 97/27559	07/1997	PCT	G06F	19/00	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

|			
Han	AN	3	Agrafiotis, D., "Theoretical Aspects of the Complex: Arts and New Technologies," *Applications and Impacts Information Processing '94*, North-Holland, Vol. II, 1994, pp. 714-719.
	AO	3	Biswas, G. *et al.*, "Evaluation of Projection Algorithms," *IEEE Transactions On Pattern Analysis And Machine Intelligence*, IEEE Computer Society, Vol. PAMI-3, No. 6, November 1981, pp. 701-708.
	AP	3	Bonchev, D. and Trinajstić, N., "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, American Institute of Physics, Vol. 67, No. 10, November 15, 1977, pp. 4517-4533.
	AQ	3	Chang, C.L. and Lee, R.C.T., "A Heuristic Relaxation Method for Nonlinear Mapping in Cluster Analysis," *IEEE Transactions on Systems, Man, and Cybernetics*, IEEE Systems, Man, and Cybernetics Society, Vol. SMC-3, March 1973, pp. 197-200.
	AR	3	Cramer, R.D. *et al.*, "Virtual Compound Libraries: A New Approach to Decision Making in Molecular Discovery Research," *Journal of Chemical Information and Computer Science*, American Chemical Society, Vol. 38, No. 6, November/December 1998, pp. 1010-1023.

EXAMINER *Hoang An Antony Nguyen Ba*	DATE CONSIDERED 5/14/04

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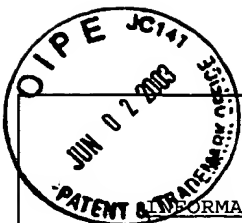
ATTY. DOCKET NO. 1503.0870001	APPLICATION NO. 09/814,160
APPLICANT Agrafiotis et al.	
FILING DATE March 22, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
Han	AA4	5,545,568	08/1996	Ellman	436	518	
	AB4	5,549,974	08/1996	Holmes	428	403	RECEIVED
	AC4	5,553,225	09/1996	Perry	395	157	
	AD4	5,565,325	10/1996	Blake	435	7.1	JUN 0 3 2003
	AE4	5,574,656	11/1996	Agrafiotis et al.	364	500	
	AF4	5,585,277	12/1996	Bowie et al.	436	518	Technology Center 2100
	AG4	5,602,755	02/1997	Ashe et al.	364	498	
	AH4	5,602,938	02/1997	Akiyama et al.	382	155	
	AI4	5,612,895	03/1997	Balaji et al.	364	496	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
Han	AJ4	WO 98/20437	05/1998	PCT	G06F	17/50	Yes No
//	AK4	WO 98/20459	05/1998	PCT	G06T	11/20	Yes No
	AL4						Yes No
	AM4						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

|			
Han	AN	4	DeMers, D. and Cottrell, G., "Non-Linear Dimensionality Reduction," *Advances in Neural Information Processing Systems*, Vol. 5, 1993, pp. 580-587.
	AO	4	Frey, P.W. and Slate, D.J., "Letter Recognition Using Holland-Style Adaptive Classifiers," *Machine Learning*, Kluwer Academic Publishers, Vol. 6, 1991, pp. 161-182.
	AP	4	Friedman, J.H., "Exploratory Projection Pursuit," *Journal of the American Statistical Association*, American Statistical Association, Vol. 82, No. 397, March 1987, pp. 249-266.
	AQ	4	Friedman, J.H. and Tukey, J.W., "A Projection Pursuit Algorithm for Exploratory Data Analysis," *IEEE Transactions on Computers*, IEEE Computer Society, Vol. C-23, No. 9, September 1974, pp. 881-889.
	AR	4	Garrido, L. *et al.*, "Use of Multilayer Feedforward Neural Nets As A Display Method for Multidimensional Distributions," *International Journal of Neural Systems*, World Scientific Publishing Co. Pte. Ltd., Vol. 6, No. 3, September 1995, pp. 273-282.

EXAMINER *Hoangan Anthony Nguyen BA*	DATE CONSIDERED 5/14/04

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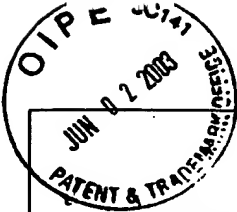
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FILING DATE March 22, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
El(au	AA5	5,634,017	05/1997	Mohanty et al.	395	326	
	AB5	5,635,598	06/1997	Lebl et al.	530	334	
	AC5	5,670,326	09/1997	Beutel	435	7.1	
	AD5	5,679,582	10/1997	Bowie et al.	436	518	
	AE5	5,684,711	11/1997	Agrafiotis et al.	364	500	
	AF5	5,703,792	12/1997	Chapman	364	496	
	AG5	5,712,171	01/1998	Zambias et al.	436	518	
	AH5	5,712,564	01/1998	Hayosh	324	210	
	AI5	5,736,412	04/1998	Zambias et al.	436	518	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ5					RECEIVED	Yes No
	AK5					JUN 0 3 2003	Yes No
	AL5					Technology Center 2100	Yes No
	AM5						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

|			
* Jlau*	AN	5	Ghose, A.K. *et al.*, "Prediction of Hydrophobic (Lipophilic) Properties of Small Organic Molecules Using Fragmental Methods: An Analysis of ALOGP and CLOGP Methods," *Journal of Physical Chemistry*, American Chemical Society, Vol. 102, No. 21, May 21, 1998, pp. 3762-3772.
	AO	5	Hall, L.H. and Kier, L.B., "The Molecular Connectivity Chi Indexes and Kappa Shape Indexes in Structure-Property Modeling," *Reviews in Computational Chemistry: Advances*, VCH Publishers, Inc., 1991, pp. 367-422.
	AP	5	Hecht-Nielsen, R., "Replicator Neural Networks for Universal Optimal Source Coding," *Science*, American Association for the Advancement of Science, Vol. 269, September 29, 1995, pp. 1860-1863.
	AQ	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Warwick and York, Inc., Vol. XXIV, No. 6, September 1933, pp. 417-441.
	AR	5	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Warwick and York, Inc., Vol. XXIV, No. 7, October 1933, pp. 498-520.

EXAMINER *Hoang ui Antony Nguyen Ba*	DATE CONSIDERED 5/14/04

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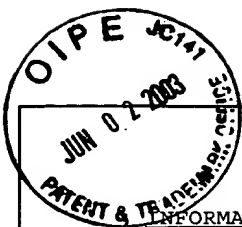
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
Han	AA6	5,740,326	04/1998	Boulet et al.	395	27	
	AB6	5,789,160	08/1998	Eaton et al.	435	6	
	AC6	5,807,754	09/1998	Zambias et al.	436	518	
	AD6	5,811,241	09/1998	Goodfellow et al.	435	7.1	
	AE6	5,832,494	11/1998	Egger et al.	707	102	
	AF6	5,858,660	01/1999	Eaton et al.	435	6	
	AG6	5,861,532	01/1999	Brown et al.	564	142	
	AH6	5,866,334	02/1999	Beutel	435	6	
	AI6	5,901,069	05/1999	Agrafiotis et al.	364	528.03	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ6						No
	AK6						Yes No
	AL6						Yes No
	AM6						Yes No

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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

Han	AN	6	Lee, R.C.T. *et al.*, "A Triangulation Method for the Sequential Mapping of Points from *N*-Space to Two-Space," *IEEE Transactions on Computers*, The Institute of Electrical and Electronics Engineers, March 1977, pp. 288-292.
	AO	6	Lipinski, C.A. *et al.*, "Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings," *Advanced Drug Delivery Reviews*, Elsevier Science B.V., Vol. 23, 1997, pp. 3-25.
	AP	6	Lobanov, V.S. and Agrafiotis, D.K., "Intelligent Database Mining Techniques," *Abstracts of Papers Part 1: 215th ACS National Meeting*, March 29-April 2, 1998, p. 19-COMP.
	AQ	6	Lobanov, V.S. *et al.*, "Rational Selections from Virtual Libraries," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 181-COMP.
	AR	6	Mao, J. and Jain, A.K., "Artificial Neural Networks for Feature Extraction and Multivariate Data Projection," *IEEE transactions on Neural Networks*, IEEE Neural Networks, Vol. 6, No. 2, March 1995, pp. 296-317.

EXAMINER *Hoang un Antony Nguyen Ba*	DATE CONSIDERED 5/14/04

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FILING DATE March 22, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
(initial)	AA7	5,908,960	06/1999	Newlander	564	177	
	AB7	5,933,819	08/1999	Skolnick et al.	706	21	
	AC7	6,014,661	01/2000	Ahlberg et al.	707	3	
	AD7	6,037,135	03/2000	Kubo et al.	435	7.24	
	AE7	6,049,797	04/2000	Guha et al.	707	6	
	AF7	6,185,506 B1	02/2001	Cramer et al.	702	19	
	AG7	5,095,443	03/1992	Watanabe	395	11	
(initial)	AH7	5,621,861	04/1997	Hayashi *et al.*	395	23	
	AI7						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ7						Yes No
	AK7						No
	AL7						Yes No
	AM7						Yes No

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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

(initial)	AN	7	Oja, E., "Principal Components, Minor Components, and Linear Neural Networks," *Neural Networks*, Pergamon Press Ltd., Vol. 5, 1992, pp. 927-935.
	AO	7	Patterson, D.E. *et al.*, "Neighborhood Behavior: A Useful Concept for Validation of 'Molecular Diversity' Descriptors," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 39, No. 16, 1996, pp. 3049-3059.
	AP	7	Pykett, C.E., "Improving the Efficiency of Sammon's Nonlinear Mapping by Using Clustering Archetypes," *Electronics Letters*, The Institute of Electrical Engineers, Vol. 14, No. 25, December 7, 1978, pp. 799-800.
	AQ	7	Rubner, J. and Tavan, P., "A Self-Organizing Network for Principal-Component Analysis," *Europhysics Letters*, European Physical Society, Vol. 10, No. 7, December 1, 1989, pp. 693-698.
	AR	7	Sadowski, J. *et al.*, "Assessing Similarity and Diversity of Combinatorial Libraries by Spatial Autocorrelation Functions and Neural Networks," *Angewandte Chemie*, VCH, Vol. 34, No. 23/24, January 5, 1996, pp. 2674-2677.

EXAMINER *(signature)*	DATE CONSIDERED 5/14/04

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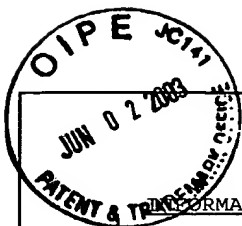
U.S. PATENT DOCUMENTS

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	AA8						
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	AH8						
	AI8						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ8						**RECEIVED** No
	AK8						**JUN 0 3 2003** No
	AL8						Technology Center 2100 No
	AM8						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

Han	AN	8	Thompson, L.A. and Ellman, J.A., "Synthesis and Applications of Small Molecule Libraries," *Chemical Reviews*, American Chemical Society, Vol. 96, No. 1, January/February 1996, pp. 555-600.
	AO	8	Barnard, John M. and Downs, Geoff M., "Computer representation and manipulation of combinatorial libraries," *Perspectives in Drug Discovery and Design*, Kluwer Academic Publishers, 1997, pp. 13-30.
	AP	8	Brint, Andrew T. and Willett, Peter, "Upperbound procedures for the identification of similar three-dimensional chemical structures," *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 2, No. 4, January 1989, pp. 311-320.
	AQ	8	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 40, No. 15, 1997, pp. 2304-2313.
	AR	8	Gillet, Valerie J. *et al.*, "The Effectiveness of Reactant Pools for Generating Structurally-Diverse Combinatorial Libraries," *Journal of Chemical Information Computer Sciences*, American Chemical Society, Vol. 37, No. 4, 1997, pp. 731-740.

EXAMINER *Hoang An G. nTony Nguyen Bn*	DATE CONSIDERED *5/14/04*

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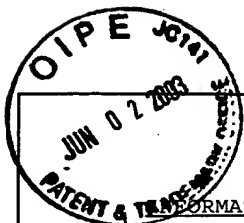
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA9						
	AB9						
	AC9						
	AD9						
	AE9						
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	AG9						
	AH9						
	AI9						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ9						Yes No
	AK9						Yes No
	AL9						Yes No
	AM9						Yes No

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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

✓ (initials)	AN	9	Gillet, Valerie J. *et al.*, "Selecting Combinatorial Libraries to Optimize Diversity and Physical Properties," *Journal of Chemical Information Computer Sciences*, American Chemical Society, Vol. 39, No. 1, 1999, pp. 169-177.
	AO	9	Kearsley, Simon K. *et al.*, "Chemical Similarity Using Physiochemical Property Descriptors," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 36, No. 1, 1996, pp. 118-127.
	AP	9	Leland, Burton A. *et al.*, "Managing the Combinatorial Explosion," *Journal of Chemical Information Computer Science*, American Chemical Society, Vol. 37, No. 1, 1997, pp. 62-70.
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	AR	9	Martin, Eric J. and Critchlow, Roger E., "Beyond Mere Diversity: Tailoring Combinatorial Libraries for Drug Discovery," *Journal of Combinatorial Chemistry*, American Chemical Society, Vol. 1, No. 1, 1999, pp. 32-45.

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FORM PTO-1449	ATTY. DOCKET NO. 1503.0870001	APPLICATION NO. 09/814,160
INFORMATION DISCLOSURE STATEMENT	APPLICANT Agrafiotis et al.	
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U.S. PATENT DOCUMENTS

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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

(examiner initials)	AN	10	Sheridan, Robert P. et al., "Chemical Similarity Using Geometric Atom Pair Descriptors," *Journal of Chemical Information Computer Sciences*, American Chemical Society, Vol. 36, No. 1, 1996, pp. 128-136.
	AO	10	Willett, Peter et al., "Chemical Similarity Searching," *Journal of Chemical Information Computer Sciences*, American Chemical Society, Vol. 38, No. 6, 1998, pp. 983-996.
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	AQ	10	Ajay et al., "Can We Learn To Distinguish between 'Drug-Like' and 'Nondrug-like' Molecules?" *Journal of Medicinal Chemistry*, 1998, American Chemical Society, Vol. 41, No. 18, pp. 3314-3324.
	AR	10	English-language Abstract of European Patent No. 0 355 628, printed from Dialog File No. 351(February, 1990 - Date of publication of application).

EXAMINER *(signature)*	DATE CONSIDERED 5/14/04

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FORM PTO-1449

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APPLICANT Agrafiotis et al.		
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Mau	AN	11	Brown, Robert D. and Martin, Yvonne C., "The Information Content of 2D and 3D Structural Descriptors Relevant to Ligand-Receptor Binding," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 1-9.
	AO	11	Brown, Robert D. and Martin, Yvonne C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1996, Vol. 36, No. 3, pp. 572-584.
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	AQ	11	*Daylight Theory: Fingerprints* (visited September 26, 2000) <http://www.daylight.com/dayhtml/doc/theory/theory.finger.html>, 9 pages.
	AR	11	*Daylight Theory: SMARTS* (visited September 26, 2000) <http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html>, 10 pages.

EXAMINER *Hoangun Anton/Nguyen Ba*	DATE CONSIDERED 5/14/04

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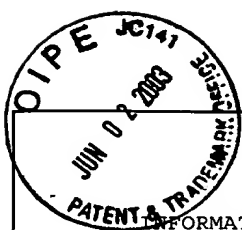
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	AO	12	Gillet, Valerie J., "Background Theory of Molecular Diversity," *Molecular Diversity in Drug Design*, Kluwer Academic Publishers, 1999, pp. 43-65.
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	AQ	12	Gorse, Dominique and Lahana, Roger, "Functional diversity of compound libraries," *Current opinion in chemical biology*, Elsevier Science Ltd., June 2000, Vol. 4, No. 3, pp. 287-294.
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EXAMINER *Hoang in Au Truy Nguyen Ba*	DATE CONSIDERED 5/14/04

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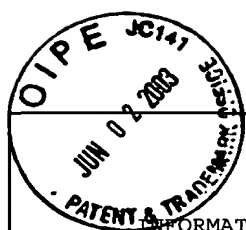
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Han	AN	13	Leach, Andrew R. *et al.*, "Implementation of a System for Reagent Selection and Library Enumeration, Profiling, and Design," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1999, Vol. 39, No. 6, pp. 1161-1172.
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	AP	13	Lobanov, Victor S. and Agrafiotis, Dimitris K., "Stochastic Similarity Selections from Large Combinatorial Libraries," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, March/April 2000, Vol. 40, No. 2, pp. 460-470.
	AQ	13	Matter, Hans and Pötter, Thorsten, "Comparing 3D Pharmacophore Triplets and 2D Fingerprints for Selecting Diverse Compound Subsets," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1999, Vol. 39, No. 6, pp. 1211-1225.
	AR	13	Matter, Hans, "Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-Dimensional and Three-Dimensional Molecular Descriptors," *Journal of Medicinal Chemistry*, American Chemical Society, 1997, Vol. 40, No. 8, pp. 1219-1229.

EXAMINER *Hoanganh Cu Tony Nguyen Br*	DATE CONSIDERED 5/14/04

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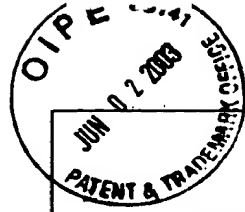
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Han	AN	14	Sadowski, Jens and Kubinyi, Hugo, "A Scoring Scheme for Discriminating between Drugs and Nondrugs," *Journal of Medicinal Chemistry*, American Chemical Society, 1998, Vol. 41, No. 18, pp. 3325-3329.
	AO	14	Schnur, Dora, "Design and Diversity Analysis of Large Combinatorial Libraries Using Cell-Based Methods," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1999, Vol. 39, No. 1, pp. 36-45.
	AP	14	Schuffenhauer, Ansgar *et al.*, "Similarity Searching in Files of Three-Dimensional Chemical Structures: Analysis of the BIOSTER Database Using Two-Dimensional Fingerprints and Molecular Field Descriptors," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 2000, Vol. 40, No. 2, pp. 295-307.
	AQ	14	Turner, David B. *et al.*, "Rapid Quantification of Molecular Diversity for Selective Database Acquisition," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, 1997, Vol. 37, No. 1, pp. 18-22.
	AR	14	Wang, Jing and Ramnarayan, Kal, "Toward Designing Drug-Like Libraries: A Novel Computational Approach for Prediction of Drug Feasibility of Compounds," *Journal of Combinatorial Chemistry*, American Chemical Society, November/December 1999, Vol. 1, No. 6, pp. 524-533.

EXAMINER	*Hoanzuu Antony Nguyen Ba*	DATE CONSIDERED 5/14/04

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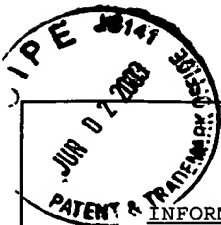|			
✓	AN	15	Gasteiger, J. *et al*, "Assessment of the Diversity of Combinatorial Libraries by an Encoding of Molecular Surface Properties," *Abstracts of Papers Part 1: 211th ACS National Meeting*, March 24-28, 1996, p. 70-CINF.
	AO	15	Hassan, Moises *et al.*, "Optimization and visualization of molecular diversity of combinatorial libraries," *Molecular Diversity*, ESCOM Science Publishers B.V., 1996, Vol. 2, pp. 64-74.
	AP	15	Bellman, R.E., *Adaptive Control Processes: A Guided Tour*, Princeton Univ. Press, Princeton, NJ (1961), entire book submitted.
	AQ	15	Bezdek, J.C., *Pattern Recognition with Fuzzy Objective Function Algorithms*, Plenum Press, New York, NY (1981), entire book submitted.
	AR	15	Johnson, M.A., and Maggiora, G.M., *Concepts and Applications of Molecular Similarity*, John Wiley and Sons, New York, NY (1990), entire book submitted.

EXAMINER	*Hoang-an Cu Tong/Nguyen BC*	DATE CONSIDERED 5/14/04

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FORM PTO-1449		ATTY. DOCKET NO. 1503.0870001		APPLICATION NO. 09/814,160
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Han	AN	16	Kohonen, T., *Self-Organizing Maps*, Springer-Verlag, Heidelberg, Germany (1995), entire book submitted.
	AO	16	Oja, E., *Subspace Methods of Pattern Recognition*, Research Studies Press, Letchworth, England (1983), entire book submitted.
	AP	16	Agrafiotis, D.K., "A New Method For Analyzing Protein Sequence Relationships Based On Sammon Maps," *Protein Science*, Cambridge University Press, Vol. 6, No. 2, February 1997, pp. 287-293.
	AQ	16	Copy of International Search Report issued October 18, 1999, for Appl. No. PCT/US99/09963, 7 pages.
	AR	16	Amzel, L.M., "Structure-based drug design," *Current Opinion in Biotechnology*, Vol. 9, No. 4, August 1998, pp. 366-369.

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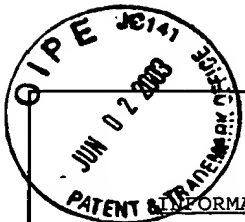
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(initialed)	AN	17	Blaney, J.M. and Martin, E.J., "Computational approaches for combinatorial library design and molecular diversity analysis," *Current Opinion in Chemical Biology*, Current Biology Ltd., Vol. 1, No. 1, June 1997, pp. 54-59.
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	AP	17	Caflisch, A. and Karplus, M., "Computational combinatorial chemistry for de novo ligand design: Review and assessment," *Perspectives in Drug Discovery and Design*, ESCOM Science Publishers B.V., Vol. 3, 1995, pp. 51-84.
	AQ	17	Danheiser, S.L., "Current Trends in Synthetic Peptide and Chemical Diversity Library Design," *Genetic Engineering News*, May 1, 1994, pp. 10 and 31.
	AR	17	Eichler, U. *et al.*, "Addressing the problem of molecular diversity," *Drugs of the Future*, Prous Science, Vol. 24, No. 2, 1999, pp. 177-190.

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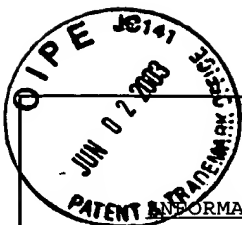
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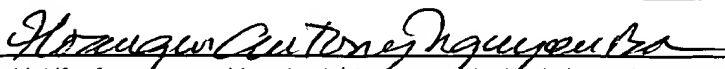
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✓	AN	18	Felder, E.R. and Poppinger, D., "Combinatorial Compound Libraries for Enhanced Drug Discovery Approaches," *Advances in Drug Research*, Academic Press, Vol. 30, 1997, pp. 112-199.
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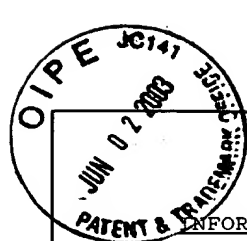
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Han	AN	19	Lajiness, M.S. *et al.*, "Implementing Drug Screening Programs Using Molecular Similarity Methods," *QSAR: Quantitative Structure-Activity Relationships in Drug Design*, Alan R. Liss, Inc., 1989, pp. 173-176.
	AO	19	Loew, G.H. *et al.*, "Strategies for Indirect Computer-Aided Drug Design," *Pharmaceutical Research*, Plenum Publishing Corporation, Vol. 10, No. 4, 1993, pp. 475-486.
	AP	19	Lynch, M.F. *et al.*, "Generic Structure Storage and Retrieval," *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 25, No. 3, August 1985, pp. 264-270.
	AQ	19	Myers, P.L. *et al.*, "Rapid, Reliable Drug Discovery," *Today's Chemist At Work*, American Chemical Society, Vol. 6, No. 7, July/August 1997, pp. 46-48, 51 & 53.
	AR	19	Pabo, C.O. and Suchanek, E.G., "Computer-Aided Model-Building Strategies for Protein Design," *Biochemistry*, American Chemical Society, Vol. 25, No. 20, 1986, pp. 5987-5991.

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Haw	AN	20	Saudek, V. *et al.*, "Solution Conformation of Endothelin-1 by H NMR, CD, and Molecular Modeling," *International Journal of Peptide Protein Res.*, Munksgaard International Publishers Ltd., Vol. 37, No. 3, 1991, pp. 174-179.
	AO	20	Singh, J. *et al.*, "Application of Genetic Algorithms to Combinatorial Synthesis: A Computational Approach to Lead Identification and Lead Optimization," *Journal of the American Chemical Society*, American Chemical Society, Vol. 118, No. 5, February 7, 1996, pp. 1669-1676.
	AP	20	Van Drie, J.H. and Lajiness, M.S., "Approaches to virtual library design," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 6, June 1998, pp. 274-283.
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	AR	20	Weber, L., "Evolutionary combinatorial chemistry: application of genetic algorithms," *Drug Discovery today*, Elsevier Science Ltd., Vol. 3, No. 8, August 1998, pp. 379-385.

EXAMINER *(signature)*	DATE CONSIDERED 5/14/04

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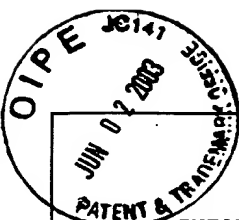
FORM PTO-1449	ATTY. DOCKET NO. 1503.0870001		APPLICATION NO. 09/814,160
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U.S. PATENT DOCUMENTS

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Haw	AN	21	Weber, L. *et al.*, "Optimization of the Biological Activity of Combinatorial Compound Libraries by a Genetic Algorithm," *Angewandte Chemie International Edition in English*, VCH, Vol. 34, No. 20, November 3, 1995, pp. 2280-2282.
	AO	21	Graybill, T.L. *et al.*, "Enhancing the Drug Discovery Process by Integration of High-Throughput Chemistry and Structure-Based Drug Design," from *Molecular Diversity and Combinatorial Chemistry: Libraries and Drug Discovery*, Chaiken and Janda (eds.), American Chemical Society, 1996, pp. 16-27.
	AP	21	Saund, E., "Dimensionality-Reduction Using Connectionist Networks," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, IEEE, Vol. 11, No. 3, March 1989, pp. 304-314.
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	AR	21	"Accelerate the Discovery Cycle with Chem-X!", Source and date of publication unclear, 2 pages.

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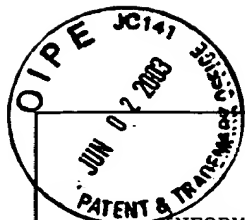
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Hoan	AN	22	Agrafiotis, D. K., "Stochastic Algorithms for Maximizing Molecular Diversity", *Journal of Chemical Information and Computer Sciences,* American Chemical Society, Vol. 37, No. 5, 1997, pp. 841-851.
	AO	22	Alsberg, B.K. *et al.*, "Classification of pyrolysis mass spectra by fuzzy multivariate rule induction-comparison with regression, *K*-nearest neighbour, neural and decision-tree methods", *Analytica Chimica Acta*, Elsevier Science B.V., Vol. 348, No. 1-3, August 20, 1997, pp. 389-407.
	AP	22	Andrea, T.A. and Kalayeh, H., "Applications of Neural Networks in Quantitative Structure-Activity Relationships of Dihydrofolate Reductase Inhibitors", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 34, No. 9, 1991, pp. 2824-2836.
	AQ	22	Aoyama, T. *et al.*, "Neural Networks Applied to Quantitative Structure-Activity Relationship Analysis", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33, No. 9, 1990, pp. 2583-2590.
	AR	22	Aoyama, T. and Ichikawa, H., "Obtaining the Correlation Indices between Drug Activity and Structural Parameters Using a Neural Network", *Chemical & Pharmaceutical Bulletin*, Pharmaceutical Society of Japan, Vol. 39, No. 2, February 1991, pp. 372-378.

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(initials)	AN	<u>23</u>	"ArQule Inc", from *http://www.bioportfolio.com/arqule/products.htm*, 5 pages, (March 18, 1998).
	AO	<u>23</u>	Baum, R.M., "Combinatorial Approaches Provide Fresh Leads for Medicinal Chemistry", *Chemical & Engineering News*, American Chemical Society, February 7, 1994, pp. 20-26.
	AP	<u>23</u>	Bentley, J. L., "Multidimensional Binary Search Trees Used for Associative Searching", *Communications of the ACM*, Association for Computing Machinery, Inc., Vol. 18, No. 9, September 1975, pp. 509-517.
	AQ	<u>23</u>	Bottou, L. and Vapnik, V. "Local Learning Algorithms", *Neural Computation*, Massachusetts Institute of Technology, Vol. 4, No. 6, November 1992, pp. 888-900.
	AR	<u>23</u>	Boulu, L.G. and Crippen, G.M., "Voronoi Binding Site Models: Calculation of Binding Modes and Influence of Drug Binding Data Accuracy", *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 10, No. 5, July/August 1989, pp. 673-682.

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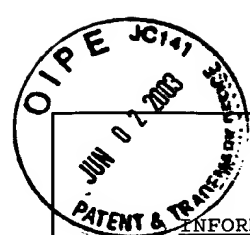
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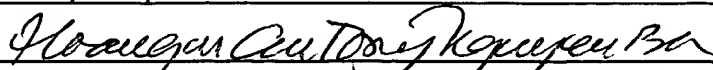
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Ham	AN	24	Boulu, L.G. *et al.*, "Voronoi Binding Site Model of a Polycyclic Aromatic Hydrocarbon Binding Protein", *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33, No. 2, 1990, pp. 771-775.
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	AP	24	Cacoullos, T., "Estimation of a Multivariate Density", *Annals of The Institute of Statistical Mathematics*, The Institute of Statistical Mathematics, Vol. 18, No. 2, 1966, pp. 179-189.
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	AR	24	Clark, D. E., and Westhead, D.R., "Evolutionary algorithms in computer-aided molecular design", *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 10, No. 4, August 1996, pp. 337-358.

EXAMINER *Hornegan Au Dony Kquepen Ba*	DATE CONSIDERED *5/14/04*

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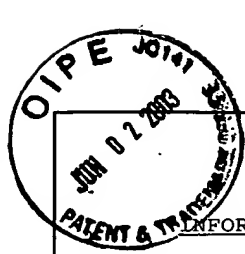
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	AN	25	Cramer, III, R. D. et al., "Comparative Molecular Field Analyisis (CoMFA). 1. Effect of Shape on Binding of Steroids to Carrier Proteins", *Journal of The American Chemical Society*, American Chemical Society, Vol. 110, No. 18, August 31, 1988, pp. 5959-5967.
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	AP	25	Crippen, G. M., "Voronoi Binding Site Models", *Journal of Computational Chemistry*, John Wiley & Sons, Inc., Vol. 8, No. 7, October/November 1987, pp. 943-955.
	AQ	25	Friedman, J. H. et al., "An Algorithm for Finding Best Matches in Logarithmic Expected Time", *ACM Transactions on Mathematical Software*, Association for Computing Machinery, Vol. 3, No. 3, September 1977, pp. 209-226.
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EXAMINER Hoang an Anthony Nguyen Ba   DATE CONSIDERED 5/14/04

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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

(examiner initials)	AN	26	Gallop, M. A. et al., "Applications of Combinatorial Technologies to Drug Discovery. 1. Background and Peptide Combinatorial Libraries", Journal of Medicinal Chemistry, American Chemical Society, Vol. 37, No. 9, April 29, 1994, pp. 1233-1251.
	AO	26	Ghose, A. K. and Crippen, G.M., "Use of Physicochemical Parameters in Distance Geometry and Related Three-Dimensional Quantitative Structure-Activity Relationships: A Demonstration Using Escherichia coli Dihydrofolate Reductase Inhibitors", Journal of Medicinal Chemistry, American Chemical Society, Vol. 28, No. 3, 1985, pp. 333-346.
	AP	26	Good, A. C. et al., "Structure-Activity Relationships from Molecular Similarity Matrices", Journal of Medicinal Chemistry, American Chemical Society, Vol. 36, No. 4, February 19, 1993, pp. 433-438.
	AQ	26	Gordon, E. M. et al., "Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic Synthesis, Library Screening Strategies, and Future Directions", Journal of Medicinal Chemistry, American Chemical Society, Vol. 37, No. 10, May 13, 1994, pp. 1385-1401.
	AR	26	Hartigan, J. A., "Representation of Similarity Matrices By Trees", Journal of the American Statistical Association, Vol. 62, No. 320, December, 1967, pp. 1140-1158.

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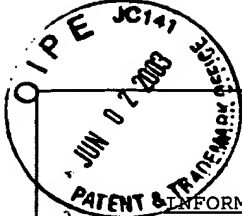
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Haw	AN	27	Hopfinger, A. J., "A QSAR Investigation of Dihydrofolate Reductase Inhibition by Baker Triazines Based upon Molecular Shape Analysis", *Journal of the American Chemical Society*, American Chemical Society, Vol. 102, No. 24, November 19, 1980, pp. 7196-7206.
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	AP	27	Kim, K. H., "Comparative molecular field analysis (CoMFA)", *Molecular Similarity in Drug Design*, ed. P. M. Dean, Blackie Academic & Professional, 1995, Ch. 12, pp. 291-331.
	AQ	27	Kohonen, T., "Self-Organized Formation of Topologically Correct Feature Maps", *Biological Cybernetics*, Springer-Verlag, Vol. 43, No. 1, 1982, pp. 59-69.
	AR	27	Koile, K. and Shapiro, R., "Building A Collaborative Drug Design System", *Proceedings of the 25h Hawaii International Conference on System Sciences*, IEEE, 1992, pp. 706-716.

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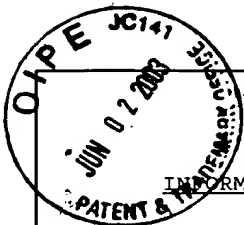
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Hau	AN	28	Kowalski, B. R. and Bender, C. F., "Pattern Recognition. II. Linear and Nonlinear Methods for Displaying Chemical Data", *Journal of the American Chemical Society*, American Chemical Society, Vol. 95, No. 3, February 7, 1973, pp. 686-693.
	AO	28	Kruskal, J. B., "Nonmetric Multidimensional Scaling: A Numerical Method", *Psychometrika*, Vol. 29, No. 2, June, 1964, pp. 115-129.
	AP	28	Lengauer, T. and Rarey, M., "Computational methods for biomolecular docking", *Current Opinion in Structural Biology*, Current Biology Ltd, Vol. 6, No. 3, June, 1996, pp. 402-406.
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	AR	28	Martin, E. J. *et al.*, "Does Combinatorial Chemistry Obviate Computer-Aided Drug Design?", *Reviews in Computational Chemistry*, VCH Publishers, Inc., Vol. 10, 1997, pp. 75-99.

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	AO	29	McMartin, C. and Bohacek, R.S., "QXP: Powerful, rapid computer algorithms for structure-based drug design", Journal of Computer-Aided Molecular Design, Kluwer Academic Publishers, Vol. 11, No. 4, July 1997, pp. 333-344.
	AP	29	Mezey, P. G. and Walker, P.D., "Fuzzy molecular fragments in drug research", Drug Discovery today, Elsevier Science Ltd., Vol. 2, No. 4, April 1997, pp. 132-137.
	AQ	29	Müller, K., "On the paradigm shift from rational to random design", Journal of Molecular Structure (Theochem), Elsevier Science B.V., Vol. 398-399, Special Issue, 1997, pp. 467-471.
	AR	29	Myers, P., "The Design Of A Universal, Informer™ Library", COMBICHEM, INC., 10 Pages, Date unknown.

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Han	AN	30	Oinuma, H. *et al.*, "Neural Networks Applied to Structure-Activity Relationships", *Journal of Medicinal Chemistry*, Vol. 33, No. 3, pp. 905-908, (1990).
	AO	30	Omohundro, S. M., "Bumptrees for Efficient Function, Constraint, and Classification Learning", *Advances in Neural Information Processing Systems 3*, Morgan Kaufmann, 1991, 7 pages, unknown.
	AP	30	Parrill, A. L., "Evolutionary and genetic methods in drug design", *Drug Discovery today*, Elsevier Science Ltd., Vol. 1, No. 12, December 1996, pp. 514-521.
	AQ	30	Polanski, J., "A neural network for the simulation of biological systems", *Journal of Molecular Structure (Theochem)*, Elsevier Science Ltd., Vol. 398-399, Special Issue, 1997, pp. 565-571.
	AR	30	Ramos-Nino, M. E. *et al.*, "A comparison of quantitative structure-activity relationships for the effect of benzoic and cinnamic acids on *Listeria monocytogenes* using multiple linear regression, artificial neural network and fuzzy systems", *Journal of Applied Microbiology*, Society for Applied Bacteriology, Vol. 82, No. 2, February 1997, pp. 168-175.

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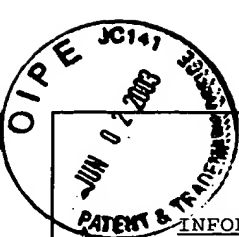
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB- CLASS	TRANSLATION
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	AL31						Yes No
	AM31						Yes No

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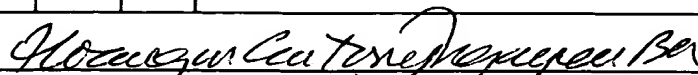
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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

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𝒪𝓁𝒻𝒶𝓂	AN	31	Rogers, D. and Hopfinger, A. J., "Application of Genetic Function Approximation to Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 34, No. 4, July/August 1994, pp. 854-866.
	AO	31	Sammon, Jr., J. W., "A Nonlinear Mapping for Data Structure Analysis", *IEEE Transactions on Computers*, IEEE, Vol. C-18, No. 5, May 1969, pp. 401-409.
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	AR	31	Specht, D. F., "A General Regression Neural Network", *IEEE Transactions on Neural Networks*, IEEE, Vol. 2, No. 6, November 1991, pp. 568-576.

EXAMINER *Horozguri Centerepegrepeei Ba*	DATE CONSIDERED 5/14/04

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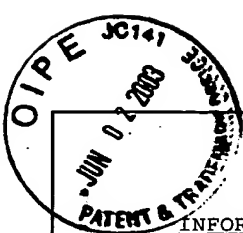
FORM PTO-1449

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO. 1503.0870001	APPLICATION NO. 09/814,160
APPLICANT Agrafiotis et al.	
FILING DATE March 22, 2001	GROUP 2122

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AJ32						Yes No
	AK32						Yes No
	AL32						Yes No
	AM32						Yes No

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Haw	AN	32	Svozil, D. *et al.*, "Neural Network Prediction of the Solvatochromic Polarity/Polarizability Parameter π^H_2", *Journal of Chemical Information and Computer Sciences*, American Chemical Society, Vol. 37, No. 2, 1997, pp. 338-342.
	AO	32	Todorov, N. P. and Dean, P. M., "Evaluation of a method for controlling molecular scaffold diversity in de novo ligand design", *Journal of Computer-Aided Molecular Design*, ESCOM Science Publishers B.V., Vol. 11, 1997, pp. 175-192.
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	AQ	32	Vapnik, V., "Principles of Risk Minimization for Learning Theory", *Advances in Neural Information Processing Systems 4*, Morgan Kaufmann Publishers, Inc., 1992, pp. 831-838.
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EXAMINER *Hozuigen Autvre Novazou Ba*	DATE CONSIDERED 5/14/04

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	AL33						Yes No
	AM33						Yes No

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	AN	33	Viswanadhan, V. N. et al., "Mapping the binding site of the nucleoside transporter protein: a 3D-QSAR study", Biochimica et Biophysica Acta, Elsevier Science Publishers B.V., Vol. 1039, No. 1, 1990, pp. 356-366.
	AO	33	Warr, W. A., "Exploiting Molecular Diversity: Small Molecule Libraries for Drug Discovery", Report of Conference held in La Jolla, California, Jan. 23-25, 1995.
	AP	33	Westhead, D. R. et al., "A comparison of heuristic search algorithms for molecular docking", Journal of Computer-Aided Molecular Design, Kluwer Academic Publishers, Vol. 11, 1997, pp. 209-228.
	AQ	33	Willett, P., "Genetic algorithms in molecular recognition and design", Trends in Biotechnology, Elsevier Science Publishers B.V., Vol, 13, No. 12, December 1995, pp. 516-521.
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EXAMINER	DATE CONSIDERED 5/14/04

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	AL34				JUN 0 3 2003		Yes No
	AM34				Technology Center 2100		Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

Haw	AN	34	Zadeh, L. A., "Communication Fuzzy Algorithms", *Information and Control*, Academic Press, Vol. 12, No. 2, February 1968, pp. 94-102.
	AO	34	Zadeh, L. A., "Fuzzy Sets", *Information and Control*, Academic Press, Vol. 8, No. 3, June 1965, pp. 338-353.
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	AQ	34	Copy of International Search Report issued May 13, 1998 for Appl. No. PCT/US97/20918, 7 pages.
	AR	34	Aoyama, T. *et al.*, "Neural Networks Applied to Structure-Activity Relationships," *Journal of Medicinal Chemistry*, American Chemical Society, Vol. 33., No. 3, 1990, pp. 905-908.

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OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

(examiner initials)	AN	35	Gasteiger, J. *et al.*, "Analysis of the Reactivity of Single Bonds in Aliphatic Molecules by Statistical and Pattern Recognition Methods," *Journal of Chemical Information Computer Sciences*, American Chemical Society, Vol. 33, No. 3, 1993, pp. 385-394.
	AO	35	Guez, A. and Nevo, I., "Neural networks and fuzzy logic in clinical laboratory computing with application to integrated monitoring," Clinica Chimica Acta, Elsevier Science Publishers B.V., Vol. 248, 1996, pp. 73-90.
	AP	35	Rouvray, D.H., "Similarity in Chemistry: Past, Present and Future," *Topics in Chemistry*, Springer-Verlag, Vol. 173, 1995, pp. 1-30.
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	AR	35	Kim, H. *et al.*, "Self-Organized Distributed Networks for Learning Highly Nonlinear Mapping," *Intelligent Engineering Systems Through Artificial Neural Networks*, American Society of Mechanical Engineers, Vol. 4, November 13-16, 1994, pp. 109-114.

EXAMINER *(signature)*	DATE CONSIDERED 5/14/04

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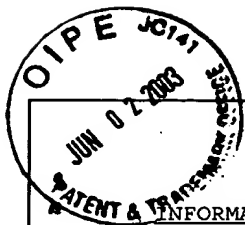
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APPLICANT Agrafiotis et al.	
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	AM36						Yes No

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Ocar	AN	36	Pal, N.R. and Eluri, V.K., "Two Efficient Connectionist Schemes for Structure Preserving Dimensionality Reduction," *IEEE Transactions on Neural Networks*, IEEE, Vol 9, No. 6, November 1998, pp. 1142-1154.
	AO	36	Domine, D. *et al.*, "Non-Linear Mapping for Structure-Activity and Structure-Property Modelling," *Journal of Chemometrics*, John Wiley & Sons, Ltd., Vol. 7, No. 4, July-August 1993, pp. 227-242.
	AP	36	Hosenpud, J. *et al.*, "The Effect of Transplant Center Volume on Cardiac Transplant Outcome: A Report of the United Network for Organ Sharing Scientific Registry," *Journal of the American Medical Association*, American Medical Association, Vol. 271, No. 23, June 15, 1994, pp. 1844-1849.
	AQ	36	Kim, J. et al., "Multiple Neural Networks Using The Reduced Input Dimension," *Proceedings of the International Conference on Acoustics, Speech, and Signal Processing (ICASSP)*, IEEE, April 19-22, 1994, pages II-601-604.
	AR	36	Copy of International Search Report issued May 28, 2002 for Appln. No. PCT/US01/08974, 7 pages.

EXAMINER *Ehrnagen Certonegrepeyou Ba*	DATE CONSIDERED 5/14/04

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